

A METHOD FOR COMPUTING LOWEST EIGENVALUES OF SYMMETRIC POLYNOMIAL DIFFERENTIAL OPERATORS BY SEMIDEFINITE PROGRAMMING

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ABSTRACT. A method for computing global minima of real multivariate polynomials based on semidefinite programming was developed by N. Z. Shor, J. B. Lasserre and P. A. Parrilo. The aim of this article is to extend a variant of their method to noncommutative symmetric polynomials in variables X and Y satisfying $YX - XY = 1$ and $X^* = X$, $Y^* = -Y$. Global minima of such polynomials are defined and showed to be equal to minima of the spectra of the corresponding differential operators. We also discuss how to exploit sparsity and symmetry. Several numerical experiments are included. The last section explains how our theory fits into the framework of noncommutative real algebraic geometry.

1. MOTIVATION

One of the most popular methods for computing global infima of real multivariate polynomials is the method of sums of squares relaxations. The idea goes back to N. Z. Shor (his original papers are summarized in [34, Chapter 9]) and it was further developed by J. B. Lasserre [13] and P. A. Parrilo [21]. See [14] for an extensive survey and [24, 8] for implementations. In this section we will present a variant of this method and in the next section we will extend it from polynomials to polynomial differential operators. Later sections are concerned with improvements of the basic method and numerical experiments.

For a given polynomial $f \in \mathbb{R}[\underline{X}]$, $\underline{X} = (X_1, \dots, X_d)$, write

$$(1) \quad \inf f := \inf\{f(x) \mid x \in \mathbb{R}^d\} = \sup\{\mu \in \mathbb{R} \mid f - \mu \geq 0 \text{ on } \mathbb{R}^d\}$$

for its unconstrained global infimum. By convention $\inf f = -\infty$ if f is not bounded from below. Note that the polynomial $X_1^2 + (1 - X_1X_2)^2$ is bounded from below but it does not attain its infimum.

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Write $\sum \mathbb{R}[\underline{X}]^2$ for the set of all sums of squares of polynomials from $\mathbb{R}[\underline{X}]$. Clearly, every element from $\sum \mathbb{R}[\underline{X}]^2$ is nonnegative on \mathbb{R}^d . In particular this is true for the polynomial $s := 1 + X_1^2 + \dots + X_d^2$. On the other hand, the Motzkin polynomial $1 + X_1^2 X_2^4 + X_1^4 X_2^2 - 3X_1^2 X_2^2$ is nonnegative on \mathbb{R}^d , $d \geq 2$, but it does not belong to $\sum \mathbb{R}[\underline{X}]^2$.

Let us consider the following sequence of approximations of $\inf f$:

$$(2) \quad \mu_k(f) := \sup\{\mu \in \mathbb{R} \mid s^k(f - \mu) \in \sum \mathbb{R}[\underline{X}]^2\},$$

where $k \in \mathbb{N} := \{0, 1, 2, \dots\}$. Since $\sum \mathbb{R}[\underline{X}]^2$ is closed in the finest locally convex topology of $\mathbb{R}[\underline{X}]$ by [29, Corollary 11.6.4], we can replace \sup by \max in (2).

Proposition 1. *If $f \in \mathbb{R}[\underline{X}]$ satisfies the following assumption:*

(*) *$f_n(x) > 0$ for every nonzero $x \in \mathbb{R}^d$ where $n = 2m$ is the total degree of f and f_n is the n -th homogeneous part of f .*

then $\lim \mu_k(f) = \inf f$.

Remark. The assumption (*) is sufficient for the existence of global infimum but it is not necessary. (A necessary condition is that $n = 2m$ and $f_n(x) \geq 0$ for every nonzero $x \in \mathbb{R}^d$.)

Proof. It is clear from (1) and (2) that $\inf f \geq \mu_k(f)$ for every k . Since $s^k(f - \mu) \in \sum \mathbb{R}[\underline{X}]^2$ implies $s^{k+1}(f - \mu) \in \sum \mathbb{R}[\underline{X}]^2$, we have by (2) that $\mu_{k+1}(f) \geq \mu_k(f)$ for every k . Finally, for every $\varepsilon > 0$, $f - \inf f + \varepsilon$ is strictly positive on \mathbb{R}^d . By Theorem 1 we can find $k_\varepsilon \in \mathbb{N}$ such that $s^{k_\varepsilon}(f - \inf f + \varepsilon) \in \sum \mathbb{R}[\underline{X}]^2$. Hence, $\mu_{k_\varepsilon}(f) \geq \inf f - \varepsilon$ by (2). \square

The following dehomogenized version of a theorem of Reznick [26] was used in the proof, see the comments after Theorem 5.5.2 in [17].

Theorem 1 (Reznick 1995). *If $f \in \mathbb{R}[\underline{X}]$ satisfies $f(x) > 0$ for every $x \in \mathbb{R}^d$ and the property (*) then $s^k f \in \sum \mathbb{R}[\underline{X}]^2$ for some $k \in \mathbb{N}$.*

Finally, we would like to convince the reader that the numbers $\mu_k(f)$ can be effectively computed. We will do so by reformulating the definition of $\mu_k(f)$ as a *semidefinite program*, i.e. an optimization problem:

$$(3) \quad \text{minimize } \text{tr}(CZ) \text{ subject to } \text{tr}(A_i Z) = b_i \text{ and } Z \geq 0$$

where C, A_i are given real symmetric matrices of the same size, b_i are given real numbers and Z is an unknown real symmetric matrix of the same size as C, A_i .

Let v_k be a vector of all monomials of total degree less or equal to $\frac{1}{2} \deg(s^k f) = k + m$. Its size is $n_k = \binom{k+m+d}{d}$. Every element of $\sum \mathbb{R}[\underline{X}]^2$ of degree $\leq 2(k + m)$ (in particular $s^k(f - \mu)$ for every $\mu \leq \mu_k(f)$) can

be written in the form $v_k^T Z v_k$ where Z is a positive semidefinite real symmetric matrix of size n_k . Therefore, by (2), we can express $\mu_k(f)$ as the solution of the following optimization problem:

$$(4) \quad \begin{aligned} &\text{Find } \mu_k(f) = \max_{\mathcal{F}} \mu \text{ where } \mathcal{F} = \{(\mu, Z) \mid \mu \in \mathbb{R}, \\ &Z \in M_{n_k}(\mathbb{R}), Z^T = Z, Z \geq 0, s^k(f - \mu) = v_k^T Z v_k\}. \end{aligned}$$

Note that (4) is not exactly a semidefinite program as defined by (3) but it can easily be converted into one by:

- eliminating μ using the linear relation obtained by comparing constant terms in $s^k(f - \mu) = v_k^T Z v_k$, (we get $f_0 - \mu = Z_{11}$ if f_0 is the constant term of f and the first component of v_k is 1),
- writing the linear relations between Z_{ij} obtained by comparing coefficients in $s^k(f - f_0 + Z_{11}) = v_k^T Z v_k$ in the form $\text{tr}(A_i Z) = b_i$,
- replacing $\mu_k(f) = \max \mu$ by $f_0 - \mu_k(f) = \min Z_{11} = \min \text{tr}(CZ)$ where $C_{11} = 1$ and other C_{ij} are 0.

Remark. Recall that the Newton polytope $N(f)$ of a polynomial $f = \sum c_\alpha X^\alpha \in \mathbb{R}[X]$ is the convex hull of its support $\{\alpha \mid c_\alpha \neq 0\}$. The main property of Newton polytopes is $N(fg) = N(f) + N(g)$. (It is proved by showing that both sets have the same extreme points, i.e. $\text{ext}N(fg) = \text{ext}N(f) + \text{ext}N(g) = \text{ext}(N(f) + N(g))$.) If $f = \sum g_i^2$, the property implies that $N(g_i) \subseteq \frac{1}{2}N(f)$ for every i . Hence, the vectors v_k from (4) need not contain all monomials of degree $\leq \frac{1}{2} \deg s^k f$ but only the monomials from $\frac{1}{2}N(s^k(f - \mu))$.

2. POLYNOMIAL DIFFERENTIAL OPERATORS

Our aim is to develop a similar theory for hermitian elements of the d -th Weyl algebra $\mathcal{W}(d)$. Recall that $\mathcal{W}(d)$ is the unital complex $*$ -algebra with generators X_k, Y_l , defining relations $Y_l X_k - X_k Y_l = \delta_{kl}$ and involution $X_k^* = X_k, Y_l^* = -Y_l$, where $k, l = 1, \dots, d$. We will write $\mathcal{W}(d)_h$ for the set of all elements $u \in \mathcal{W}(d)$ such that $u^* = u$ and $\sum \mathcal{W}(d)^2$ for the set of all finite sums of elements $u^* u$ where $u \in \mathcal{W}(d)$.

The Schrödinger representation π_0 is the $*$ -representation of $\mathcal{W}(d)$ acting on the Schwartz space $\mathcal{S}(\mathbb{R}^d)$ considered as dense domain of $L^2(\mathbb{R}^d)$, which is defined by $(\pi_0(X_k)\phi)(t) = t_k \phi(t)$ and $(\pi_0(Y_l)\phi)(t) = \frac{\partial \phi}{\partial t_l}(t)$ for $k, l = 1, \dots, d$. We will write $\mathcal{W}(d)_+$ for the set of all elements $u \in \mathcal{W}(d)_h$ such that $\langle \pi_0(u)\phi, \phi \rangle \geq 0$ for all $\phi \in \mathcal{S}(\mathbb{R}^d)$. Clearly, $\sum \mathcal{W}(d)^2 \subseteq \mathcal{W}(d)_+$ while the converse is false by [30, Section 6].

For a given element $c \in \mathcal{W}(d)_h$ write

$$(5) \quad \inf c := \sup \{ \lambda \in \mathbb{R} \mid c - \lambda \cdot 1 \in \mathcal{W}(d)_+ \}$$

if $\pi_0(c)$ is bounded from below. Otherwise write $\inf c = -\infty$. Clearly, $\inf c$ is equal to the infimum of the numerical range of $\pi_0(c)$, i.e.

$$\inf c = \inf \{ \langle \pi_0(c)v, v \rangle \mid v \in \mathcal{S}(\mathbb{R}^d), \|v\| = 1 \}.$$

When $\pi_0(c)$ is bounded from below, one can define the Friedrichs extension $\pi_0(c)_F$ of $\pi_0(c)$ and show that

$$\inf c = \min \sigma(\pi_0(c)_F),$$

see e.g. [16] and the references therein. If $\sigma(\pi_0(c)_F)$ is also discrete then $\inf c$ is equal to the lowest eigenvalue of $\pi_0(c)_F$.

Remark. There are well-known sufficient conditions on $V(X)$ implying that the Schrödinger operator $L = \pi_0(-\sum_{i=1}^d Y_i^2 + V(X))$ is bounded from below, is essentially selfadjoint (i.e. L_F is the only selfadjoint extension of L) and has discrete spectrum, see [20, Sections 8.1, 8.2].

Let c be an element of $\mathcal{W}(d)_h$ of even total degree $\deg c$. We propose the following method for computing $\inf c$. Firstly, pick a sequence $s = (s_k)_{k \in \mathbb{N}}$ of elements of $\mathcal{W}(d)$ with $s_0 = 1$. Secondly, solve the following sequence of “semidefinite programs”:

$$(6) \quad \begin{aligned} &\text{Find } \mu_k(c, s) = \max_{\mathcal{F}} \mu \text{ where } \mathcal{F} = \{(\mu, Z) \mid \mu \in \mathbb{R}, \\ &Z \in M_{n_k}(\mathbb{C}), Z^H = Z, Z \geq 0, b_k^*(c - \mu)b_k = v_k^H Z v_k\} \end{aligned}$$

where for every $k \in \mathbb{N}$, $b_k = \prod_{i=0}^k s_i$, v_k is a vector of all monomials m in the generators of $\mathcal{W}(d)$ such that $\deg m \leq \frac{1}{2} \deg b_k^* c b_k = \deg b_k + \frac{1}{2} \deg c$ and n_k is the size of v_k .

Clearly, $\mu_{k+1}(c, s) \geq \mu_k(c, s)$ for every k since b_k divides b_{k+1} in (6). If $\pi_0(s_k)$ is invertible for every k , then, by (5) and (6), the sequence $\mu_k(c, s)$ is bounded above by $\inf c$. The main question is what additional assumptions on c and s are needed to ensure that $\lim \mu_k(c, s) = \inf c$. Our numerical experiments suggest that the only additional assumption required is that s_k are nonconstant but we are unable to prove that. What we can prove about convergence is summarized in Propositions 2 and 3 below; see also Conjecture 1.

Recall that *the leading symbol* of an element

$$c = \sum_{\alpha, \beta \in \mathbb{N}^d} c_{\alpha, \beta} X^\alpha Y^\beta = \sum_{k=0}^{\deg c} \sum_{\substack{\alpha, \beta \in \mathbb{N}^d \\ |\alpha| + |\beta| = k}} c_{\alpha, \beta} X^\alpha Y^\beta \in \mathcal{W}(d)$$

(in multiindex notation) is the element

$$\bar{c} = \sum_{\substack{\alpha, \beta \in \mathbb{N}^d \\ |\alpha| + |\beta| = \deg c}} c_{\alpha, \beta} X^\alpha \xi^\beta \in \mathbb{C}[X, \xi].$$

If $c = c^*$, then $\bar{c}(X, i\xi) \in \mathbb{R}[X, \xi]$. For example, the leading symbol of $N := \sum_{i=1}^d \frac{1}{2} (X_i^2 - Y_i^2 - 1) \in \mathcal{W}(d)_h$ is $\bar{N} = \sum_{i=1}^d \frac{1}{2} (X_i^2 - \xi_i^2)$. Note that $\bar{N}(X, i\xi) = \sum_{i=1}^d \frac{1}{2} (X_i^2 + \xi_i^2)$ is > 0 if $(X, \xi) \neq (0, 0)$.

Proposition 2. *Suppose that $c \in \mathcal{W}(d)_h$, $4 \mid \deg c$ and $\bar{c}(X, i\xi) > 0$ for every $X, \xi \in \mathbb{R}^d$ with $(X, \xi) \neq (0, 0)$. Pick $\alpha \in \mathbb{R}^+ \setminus \mathbb{N}$ and a sequence $m_k \in \mathbb{Z}$ in which every integer appears infinitely many times and write $s_0 = 1$, $s_k = N + (m_k + \alpha) \cdot 1$ for $k \geq 1$. Then $\lim \mu_k(c, s) = \inf c$.*

This is an immediate consequence of the fact that $\sigma(N) = \mathbb{N}$ and the following result of Schmüdgen which is a noncommutative analogue of Theorem 1. (Assumption (1) can be relaxed slightly, see [19, Th. 1.2], but this does not help us here.)

Theorem 2. [30, Th. 1.1] *Suppose $c \in \mathcal{W}(d)_h$, $\deg c = 2m$, satisfies*

- (1) *There exists $\varepsilon > 0$ such that $c - \varepsilon \cdot 1 \in \mathcal{W}(d)_+$.*
- (2) *$\bar{c}(X, i\xi) > 0$ for every $X, \xi \in \mathbb{R}^d$ with $(X, \xi) \neq (0, 0)$.*

Finally, fix $\alpha \in \mathbb{R}^+ \setminus \mathbb{N}$ and write \mathcal{N} for the set of all finite products of elements $N + (\alpha + n) \cdot 1$, where $n \in \mathbb{Z}$.

If m is even, then there exists $b \in \mathcal{N}$ such that $bc b \in \sum \mathcal{W}(d)^2$. If m is odd, then there exists $b \in \mathcal{N}$ such that $\sum_{j=1}^d b(X_j + Y_j)c(X_j - Y_j)b \in \sum \mathcal{W}(d)^2$.

Proposition 3 is a variant of Proposition 2. We need some notation. We assume that $d = 1$ and write $q = X$ and $p = -iY$. Every nonzero $c \in \mathcal{W}(1)$ can be uniquely expressed as

$$c = \sum_{j=0}^{d_1} \sum_{l=0}^{d_2} \gamma_{jl} p^j q^l = \sum_{n=0}^{d_2} f_n(p) q^n = \sum_{k=0}^{d_1} g_k(q) p^k,$$

where $f_{d_2} \neq 0$ and $g_{d_1} \neq 0$. In this case we say that c has multidegree (d_1, d_2) . We fix two nonzero reals α and β . Let \mathcal{S} be the monoid generated by $s_1 = p - \alpha i$, $s_2 = q - \beta i$ and s_1^* , s_2^* . It is an Ore set.

Proposition 3. *Suppose that $c \in \mathcal{W}(1)_h$ has multidegree $(2m_1, 2m_2)$, where $m_1, m_2 \in \mathbb{N}$, $\gamma_{2m_1, 2m_2} \neq 0$ and f_{2m_2} and g_{2m_1} are positive on the real line. Since \mathcal{S} is countable we can number its elements, say $(u_i)_{i \in \mathbb{N}}$, assuming $u_0 = 1$. Write $s_0 = 1$ and let, for every $k \geq 0$, $s_{k+1} \in \mathcal{S}$ be the common right multiple of s_k and u_{k+1} that exists by the Ore property. Then $\lim \mu_k(c, s) = \inf c$.*

This is an immediate consequence of the following result of Schmüdgen:

Theorem 3. [33, Theorem 5]. *Let c be a nonzero hermitian element of $\mathcal{W}(1)$ of multidegree $(2m_1, 2m_2)$, where $m_1, m_2 \in \mathbb{N}$. Suppose that:*

- (1) *There exists a bounded self-adjoint operator $T > 0$ on $L^2(\mathbb{R})$ such that $\pi_0(c) \geq T$.*
- (2) *$\gamma_{2m_1, 2m_2} \neq 0$ and f_{2m_2} and g_{2m_1} are positive on the real line.*

*Then there exists an element $s \in \mathcal{S}$ such that $s^*cs \in \sum \mathcal{W}(1)^2$.*

Note that neither Proposition 2 nor Proposition 3 cover Schrödinger operators $-Y^2 + V(X)$ with polynomial potential $V(X)$ of degree > 2 . This case however fits into the following conjecture:

Conjecture 1. *Suppose that $c \in \mathcal{W}(1)_h$ is bounded from below and $s_k = aX + i1$ for every $k \in \mathbb{N}$. Then $2|\deg c$ and $\lim \mu_k(c, s) = \inf c$.*

This conjecture is true if the following claim from [10] is true:

Claim. *Let \mathcal{A} be the algebra obtained from $\mathcal{W}(1)$ with the addition of the generator $(aX + i1)^{-1}$ (for $a \in \mathbb{R}$) and the commutation relation $[p, (aX + i1)^{-1}] = ia(aX + i1)^{-2}$. Then every positive element $c \in \mathcal{A}$ has a quadratic sum factorization $c = \sum d_k^* d_k$ for some finite set of elements $d_k \in \mathcal{A}$.*

The proof in [10] seems to have a gap (where they use a result of Schmüdgen).

3. IMPLEMENTATION, NUMERICAL EXAMPLES FOR $d = 1$

The computation of $\mu_k(c, s)$ was implemented as follows. Firstly, the input for semidefinite programs (i.e. the matrices C, A_i and the numbers b_i) was computed by Mathematica[®] (Wolfram Research) in rational (i.e. exact) arithmetics. Linear relations among Z_{ij} had to be solved before they were converted into the form $\text{tr}(A_i Z) = b_i$ to ensure that the matrices A_i were linearly independent. Secondly, the input data was exported to Matlab[®] (Mathworks) where it was solved by either SeDuMi [35] or SDPT3 [36] semidefinite programming solver (through the Yalmip interface [15]) in floating point arithmetics.

The problems of the basic method are illustrated by the following toy example in $d = 1$:

Example 1. Write $c = (2N + 1)^2 = (X^2 - Y^2)^2$. Clearly, $\inf c = 1$ but pretend we don't know that. The element c satisfies the assumptions of Proposition 2. We fix $\alpha = \frac{1}{2}$ and $s_k = N + \alpha \cdot 1$. We will compute approximations $\mu_0(c, s), \dots, \mu_3(c, s)$ of $\inf c$ using sedumi and sdpt3 respectively. The results are in Table 1. The first approximation is very good but higher approximations are getting worse while the theory says they should be getting better.

k	$\mu_k(c, s)$ (sedumi)	$\mu_k(c, s)$ (sdpt3)	n_k	m_k
0	0.999999999760	0.9999999993360	6	15
1	1.000044013288	0.999999989593	15	45
2	1.112894824977	0.999999941936	28	91
3	73.69340728792	24.89729311234	45	153

TABLE 1. The table of Example 1. The numbers n_k and m_k refer to the size and number of matrices A_i in semidefinite programs used for computing $\mu_k(c, s)$.

The lesson that we learn is that semidefinite programs should be kept as small as possible. The most natural way to do this is to exploit sparsity. (Later we will also discuss how to exploit symmetry.) For every

$$c = \sum c_{\alpha, \beta} X^\alpha Y^\beta \in \mathcal{W}(1)$$

write $N'(c)$ for the convex hull of the set

$$\bigcup_{\substack{\alpha, \beta \in \mathbb{N} \\ c_{\alpha, \beta} \neq 0}} \{(\alpha - k, \beta - k) \mid k = 0, \dots, \min(\alpha, \beta)\}.$$

The point is that because of the relation $YX - XY = 1$ we must replace $\{(\alpha, \beta)\}$ by $\{(\alpha - k, \beta - k) \mid k = 0, \dots, \min(\alpha, \beta)\}$. As outlined in Section 1, one can prove the property $N'(fg) = N'(f) + N'(g)$ for every $f, g \in \mathcal{W}(1)$. The property implies that the vectors v_k from the definition of $\mu_k(c, s)$ need not contain all monomials $X^\alpha Y^\beta$ with $\alpha + \beta \leq \deg b_k^* f b_k$ but only those from $\frac{1}{2}N'(b_k^*(c - \mu)b_k)$. This method works particularly well if b_k depend only on X .

Example 2. Let $\lambda_0(\beta)$ be the lowest eigenvalue of $\pi_0(c_\beta)$ where

$$c_\beta = -Y^2 + X^2 + \beta X^4.$$

The values of $\lambda_0(\beta)$ for various β were computed in [2, Table 1] to 15 decimals. We refer to his values as “exact”.

Let $\mu_k(\beta)$ be the solution of the semidefinite program (6) for $c = c_\beta$, $b_k = (i - X)^k$ and $v_k = (1, X, \dots, X^{k+2}, Y, XY, \dots, X^k Y)^T$. For each $\beta \in \{0.0001, 1, 10000\}$ and $k = 0, 1, \dots, 14$, we will compute $\mu_k(\beta)$ by sdpt3. Finally, for each β we draw the semi-log plot of the sequence of relative errors of $\mu_k(\beta)$ with respect to $\lambda_0(\beta)$, i.e. the plot of the sequence $k \mapsto \log_{10} \left| \frac{\lambda_0(\beta) - \mu_k(\beta)}{\lambda_0(\beta)} \right|$. The results are presented in Figure 1. In theory these plots should decrease to $-\infty$. By Figure 1, they decrease only during first 8-10 steps. Similar results are obtained for $b_k = (1 + X^2)^k$ and $v_k = (1, X, \dots, X^{2k+2}, Y, \dots, X^{2k} Y)^T$, see Figure 2.

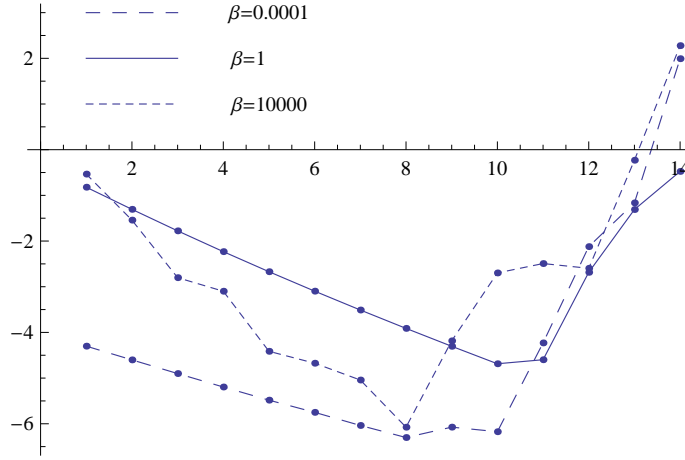


FIGURE 1. The plots of $k \mapsto \log_{10} \left| \frac{\lambda_0(\beta) - \mu_k(\beta)}{\lambda_0(\beta)} \right|$ for $c = -Y^2 + X^2 + \beta X^4$, $s_k = i - X$ and sparse v_k (Example 2)

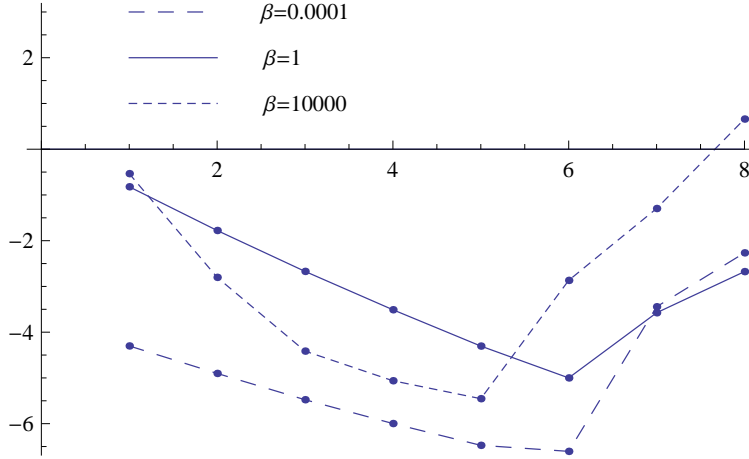


FIGURE 2. The plots of $k \mapsto \log_{10} \left| \frac{\lambda_0(\beta) - \mu_k(\beta)}{\lambda_0(\beta)} \right|$ for $c = -Y^2 + X^2 + \beta X^4$, $s_k = 1 + X^2$ and sparse v_k (Example 2)

Whatever improvement we use, things eventually start to go wrong (because of rounding errors) and the question is when to stop. If we use `sdpt3`, wrong values tend to undershoot, while if we use `sedumi`, they tend to overshoot. We can use this observation to formulate an empirical stopping criterium for `sdpt3`: If $\mu_0 < \mu_1 < \dots < \mu_l > \mu_{l+1}$, then return μ_l as the best approximation for the lowest eigenvalue. We can also use $\min(\mu_l - \mu_{l-1}, \mu_l - \mu_{l+1})$ as an estimate of its precision. There is no such stopping criterium for `sedumi`. We will use only `sdpt3` in the sequel.

Remark. Another trick that sometimes improves stability in the commutative case is scaling $X \rightarrow \lambda X$, $Y \rightarrow \lambda Y$. In our case this does not work, because it violates the relation $YX - XY = 1$. On the other hand, the transformation $X \rightarrow \lambda X$, $Y \rightarrow \lambda^{-1}Y$ respects the relation but it does not improve stability.

4. EXPLOITING SYMMETRY - FINITE GROUPS

Suppose that G is a finite group acting on \mathbb{R}^d by orthogonal transformations. This action induces in a natural way an action ρ on the polynomial ring $\mathbb{R}[\underline{X}]$ and an action σ on symmetric matrices that appear in our semidefinite programs, see [5]. The action σ helps us put the matrices in our semidefinite programs into block diagonal form and thus reduce the amount of computation. It follows that every G -invariant sum of squares is a sum of squares of invariant and semi-invariant polynomials, see [5, Theorem 5.3].

The same theory also works for Weyl algebras and even some more general algebras, such as enveloping algebras of Lie algebra. Finite generation of the ring of invariants for this situation was established in [4] by passing to the corresponding graded ring. An extension of [5, Theorem 5.3] to locally finite-dimensions actions of compact groups by $*$ -automorphisms is provided by the last equation in the proof of [28, Proposition 4].

Example 3. We would like to approximate the lowest eigenvalue of

$$L = \pi_0(Y^4 + X^4)$$

by exploiting symmetry. Let $G = \{1, i, -1, -i\}$ act on $\mathcal{W}(1)$ by

$$\rho(i)(X) = iY \quad \text{and} \quad \rho(i)(Y) = iX.$$

Clearly, $\rho(L) = L$. Since $\rho(i)(X + Y) = i(X + Y)$ and $\rho(i)(X - Y) = -i(X - Y)$, it is more convenient to work with the generators

$$a = \frac{X + Y}{\sqrt{2}} \quad \text{and} \quad a^* = \frac{X - Y}{\sqrt{2}}.$$

We start with the zero-th approximation, i. e. we would like to find the largest μ_0 such that $Y^4 + X^4 - \mu_0 \cdot 1$ is a sum of hermitian squares. We have to consider the 6-dimensional space M_2 of all monomials of degree less or equal to 2. Eigenvectors of the restriction of ρ to M_2 are:

$$\begin{aligned} \lambda_1 = 1 : & \quad 1, a^*a \\ \lambda_2 = -1 : & \quad a^2, (a^*)^2 \\ \lambda_3 = i : & \quad a, \\ \lambda_4 = -i : & \quad a^*. \end{aligned}$$

The 6×6 matrices that appear in our semidefinite program can therefore be assumed to be block diagonal with two 2×2 blocks and two 1×1 blocks. We have therefore reduced the number of variables from 15 to 8. Using `sdpt3`, we get

$$\mu_0 = 1.328427121$$

To compute higher approximations, we need appropriate denominators b_k such that $b_k^* L b_k$ is still G -invariant. Clearly, we can take for b_k every G -semiinvariant polynomial, e.g. any element from \mathcal{N} . For

$$b_k = (2N + 1)^k = (X^2 - Y^2)^k = (2a^*a + 1)^k$$

we get

$$\mu_1 = 1.396727721$$

using the eigenvectors

$$\begin{aligned} \lambda_1 = 1 : & \quad 1, a^*a, a^4, (a^*)^4, (a^*)^2a^2 \\ \lambda_2 = -1 : & \quad a^2, (a^*)^2, a^*a^3, (a^*)^3a \\ \lambda_3 = i : & \quad a, (a^*)^3, a^*a^2 \\ \lambda_4 = -i : & \quad a^*, a^3, (a^*)^2a \end{aligned}$$

and

$$\mu_2 = 1.396726593$$

using the eigenvectors

$$\begin{aligned} \lambda_1 = 1 : & \quad 1, a^*a, a^4, (a^*)^4, (a^*)^2a^2, (a^*)^5a, (a^*)^3a^3, a^*a^5 \\ \lambda_2 = -1 : & \quad a^2, (a^*)^2, a^*a^3, (a^*)^3a, a^6, (a^*)^2a^4, (a^*)^4a^2, (a^*)^6 \\ \lambda_3 = i : & \quad a, (a^*)^3, a^*a^2, (a^*)^4a, (a^*)^2a^3, a^5 \\ \lambda_4 = -i : & \quad a^*, a^3, (a^*)^2a, a^*a^4, (a^*)^3a^2, (a^*)^5 \end{aligned}$$

Our stopping criterium tells us that μ_1 is likely the best approximation we can get by this choice of b_k . The method based on Conjecture 1 gives $\mu'_4 = 1.396718666$, $\mu'_5 = 1.396726819$, $\mu'_6 = 1.396718409$, i.e. a similar approximation and a similar estimate for precision.

5. A CONJECTURE ABOUT RADIAL DIFFERENTIAL OPERATORS

For every integer $d \geq 1$, we can identify the Hilbert space $L^2(\mathbb{R}^+; r^{d-1})$ with the subspace of $L^2(\mathbb{R}^d)$ consisting of radially invariant functions. Let $\mathcal{S}_d(\mathbb{R}^+)$ be the subspace of $L^2(\mathbb{R}^+; r^{d-1})$ which corresponds to the space of radially invariant Schwartz functions on \mathbb{R}^d . Let π_d be the representation of the first Weyl algebra $\mathcal{W}(1)$ which acts on $\mathcal{S}_d(\mathbb{R}^+)$ by

$$(\pi_d(X)f)(r) = rf(r) \text{ and } (\pi_d(Y)f)(r) = f'(r).$$

This representation is not a $*$ -representation however if we consider the standard involution on $\mathcal{W}(1)$ and the adjoint operation $L \mapsto L^+$ on

differential operators. To make it a $*$ -representation we must consider a new involution $L \mapsto L^* := r^{d-1}L^+r^{1-d}$ which is conjugate to $L \mapsto L^+$.

The aim of this section is to provide numerical support for the following conjecture:

Conjecture 2. *If $c \in \mathcal{W}(1)_h$ is such that $\pi_d(c) > 0$ for some d then $\deg_Y c$ is even and there exist $k \in \mathbb{N}$ and finitely many $g_i, h_j \in \mathcal{W}(1)$ such that*

$$(1 + X^2)^k c (1 + X^2)^k = \sum_i g_i^* g_i + \sum_j h_j^* X h_j.$$

Suppose we want to compute the lowest eigenvalue λ_0 of a d -dimensional radially invariant Schrödinger operator

$$L = -\frac{1}{r^{d-1}} \frac{d}{dr} (r^{d-1} \frac{d}{dr}) + V(r)$$

where $V(r)$ is a real polynomial in r and $1/r$. Pick the smallest $m \in \mathbb{N}$ such that $r^{2m+d-1}V(r)$ has no negative powers. Conjecture 2 implies that the following sequence converges to λ_0 :

$$(7) \quad \mu_k := \sup\{\mu \in \mathbb{R} \mid \exists g_i, h_j \in \mathcal{W}(1) : (1 + X^2)^k (-X^m Y X^{d-1} Y X^m + X^{2m+d-1}(V(X) - \mu))(1 + X^2)^k = \sum_i g_i^* g_i + \sum_j h_j^* X h_j\}.$$

We can write $g_i^* g_i + \sum_j h_j^* X h_j = u_k^* A u_k + v_k^* (X B) v_k$, where u_k, v_k are suitable vectors of monomials and A, B are positive semidefinite complex hermitian matrices. Therefore, we can rewrite the definition of μ_k as a semidefinite program.

Example 4. For $d = 1, \dots, 10$ and

$$V(r) = r + r^2 + r^3,$$

we will compute approximations μ_0, \dots, μ_5 of λ_0 using

$$u_k = \begin{cases} (1, X, \dots, X^{2k+1+\frac{d-1}{2}}, Y, \dots, X^{2k+\frac{d-1}{2}} Y)^T & d \text{ odd,} \\ (1, X, \dots, X^{2k+1+\frac{d}{2}})^T & d \text{ even.} \end{cases}$$

and

$$v_k = \begin{cases} (1, X, \dots, X^{2k+1+\frac{d-1}{2}})^T & d \text{ odd,} \\ (1, X, \dots, X^{2k+\frac{d}{2}}, Y, \dots, X^{2k-1+\frac{d}{2}} Y)^T & d \text{ even.} \end{cases}$$

and compare them with [6, Table 1]. The results are in Table 2.

There is a problem with $d = 1$. Namely, by [6, Table 1], λ_0 is approximately 1.8306, while we can show (in exact arithmetics) that μ_0 is approximately 1.9051. A possible explanation is that the eigenfunction corresponding to 1.8306 is not in $L^2(\mathbb{R}^+)$. This has nothing to do with Conjecture 2.

d	exact	μ_0	μ_1	μ_2	μ_3	μ_4	μ_5
2	3.5644	3.4973	3.5623	3.5643	<u>3.5644</u>	3.5643	3.5630
3	5.3066	5.2277	5.3046	<u>5.3065</u>	5.3064	5.3058	5.3034
4	7.0746	7.0073	7.0730	<u>7.0746</u>	7.0746	7.0677	7.0405
5	8.8720	8.8187	8.8709	<u>8.8720</u>	8.8720	8.8717	8.8713
6	10.6987	10.6488	10.6978	<u>10.6986</u>	10.6986	10.6874	10.6030
7	12.5534	12.5337	12.5523	12.5534	<u>12.5534</u>	12.5533	12.5530
8	14.4348	14.4229	14.4345	<u>14.4348</u>	14.4342	14.3901	14.0928
9	16.3415	16.3338	16.3413	<u>16.3414</u>	16.3414	16.3414	16.3411
10	18.2720	18.2664	18.2719	<u>18.2720</u>	18.2712	18.2041	16.5905

TABLE 2. The table of Example 4. For each d , the best approximation is underlined. Exact values for λ_0 are from [6, Table 1].

λ	exact	μ_0	μ_1	μ_2	μ_3	μ_4	μ_5
0.0	2.3381	1.8899	2.3193	2.3368	<u>2.3380</u>	2.3300	2.2971
0.2	2.1673	1.7277	2.1490	2.1661	<u>2.1672</u>	2.1582	2.1198
0.4	1.9885	1.5583	1.9706	1.9874	<u>1.9884</u>	1.9783	1.9372
0.6	1.8011	1.3810	1.7838	1.8001	<u>1.8010</u>	1.7898	1.7349
0.8	1.6044	1.1951	1.5878	1.6035	<u>1.6043</u>	1.5915	1.5447
1.0	1.3979	1.0000	1.3820	1.3971	<u>1.3978</u>	1.3832	1.3280
1.2	1.1808	0.7949	1.1657	1.1801	<u>1.1807</u>	1.1641	1.0800
1.4	0.9526	0.5790	0.9383	0.9520	<u>0.9525</u>	0.9360	0.8712
1.6	0.7127	0.3516	0.6992	0.7121	<u>0.7124</u>	0.6937	0.6241
1.8	0.4603	0.1119	0.4476	0.4597	<u>0.4599</u>	0.4374	0.3691

TABLE 3. The table of Example 5. For each λ , the best approximation is underlined. Exact values for λ_0 (rounded from 15 to 4 decimals) are from [11, Table I].

Example 5. Suppose that $d = 1$ and

$$V(r) = -\frac{\lambda}{r} + r.$$

We will compute approximations μ_0, \dots, μ_5 of the lowest eigenvalue using $u_k = (1, \dots, X^{2k+1}, Y, \dots, X^{2k+1}Y)^T$ and $v_k = (1, \dots, X^{2k+1})^T$ and compare them with [11, Table I]. The results are in Table 3.

Example 6. Suppose that $d = 1$ and

$$V(r) = ar^2 + \frac{b}{r^2}$$

where $a > 0$, $b > -\frac{1}{4}$. We apply one step of our method and divide the result by r on both sides. We get

$$-\frac{d^2}{dr^2} + V(r) - 2\sqrt{a}(1 + \sqrt{b + \frac{1}{4}}) = g^*g,$$

where $g = \frac{d}{dr} + \sqrt{a}r - (\frac{1}{2} + \sqrt{b + \frac{1}{4}})r^{-1}$, which implies the inequality

$$\lambda_0 \geq 2\sqrt{a}(1 + \sqrt{b + \frac{1}{4}}).$$

Similarly, if $d = 1$ and

$$V(r) = \frac{a}{r} + \frac{b}{r^2}$$

where $a < 0$, $b > -\frac{1}{4}$, then we get as above

$$-\frac{d^2}{dr^2} + V(r) + \frac{a^2}{(1 + 2\sqrt{b + \frac{1}{4}})^2} = h^*h,$$

where $h = \frac{d}{dr} - \frac{a}{1 + 2\sqrt{b + \frac{1}{4}}} - (\frac{1}{2} + \sqrt{b + \frac{1}{4}})r^{-1}$, hence

$$\lambda_0 \geq -\frac{a^2}{(1 + 2\sqrt{b + \frac{1}{4}})^2}.$$

It is shown in [9] that both inequalities for λ_0 are in fact equalities but this is not clear from our method. If $a \geq 0$ in the second case then $\lambda_0 \geq 0$ because

$$-\frac{d^2}{dr^2} + V(r) = \frac{a}{r} + \left(\frac{d}{dr} - \frac{\frac{1}{2} + \sqrt{b + \frac{1}{4}}}{r}\right)^* \left(\frac{d}{dr} - \frac{\frac{1}{2} + \sqrt{b + \frac{1}{4}}}{r}\right).$$

6. OTHER *-ALGEBRAS

The aim of this short section is to outline a possible extension of our theory from $\mathbb{R}[\underline{X}]$ and $\mathcal{W}(d)$ to other *-algebras.

Let A be a finitely generated real or complex unital *-algebra and \mathcal{R} a family of equivalence classes of irreducible (possibly unbounded) *-representations of A . We can consider the elements of A as “polynomials” and elements of \mathcal{R} as (evaluations in) “points”, see [32]. For every element $c \in A$ such that $c^* = c$ we can define

$$\inf c := \sup\{\mu \in \mathbb{R} \mid \pi(c - \mu \cdot 1) \geq 0 \text{ for every } \pi \in \mathcal{R}\}.$$

Clearly, our method for computing $\inf c$ can be applied to A if:

- the monomials in the generators are linearly independent and
- it satisfies an analogue of Theorem 1.

Examples of such algebras are:

- algebras of matrix polynomials [1],
- enveloping algebras of finite dimensional real Lie algebras [31],
- algebras of trigonometric polynomials [18],
- finitely generated free real algebras [7], [12] (also [23], [3]).

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REFERENCES

- [1] C.-G. Ambrozie, F.-H. Vasilescu, Operator-theoretic positivstellensätze, *Z. Anal. Anwendungen* **22** (2003), no. 2, 299–314.
- [2] K. Banerjee, General anharmonic oscillators, *Proc. R. Soc. Lond. A.* **364** (1978), 265–275.
- [3] S. Burgdorf and I. Klep, The truncated tracial moment problem, *arXiv:1001.3679v1*.
- [4] L. Chiang, H. Chu, M. Kang, Generation of invariants, *J. Algebra* **221** (1999), no. 1, 232–241.
- [5] K. Gatermann, P. A. Parrilo, Symmetry groups, semidefinite programs, and sums of squares, *J. Pure Appl. Algebra* **192** (2004), no. 1-3, 95–128.
- [6] R. L. Hall, N. Saad, Bounds on Schrödinger eigenvalues for polynomial potentials in N dimensions, *J. Math. Phys.* **38** (1997), 4909–4913.
- [7] J. W. Helton, “Positive” noncommutative polynomials are sums of squares, *Ann. of Math. (2)* **156** (2002), no. 2, 675–694.
- [8] D. Henrion, J.-B. Lasserre, GloptiPoly: global optimization over polynomials with Matlab and SeDuMi, *ACM Trans. Math. Software* **29** (2003), no. 2, 165–194.
- [9] S. M. Ikhdaïr and R. Sever, On solutions of the Schrödinger equation for some molecular potentials: wave function ansatz, *Cent. Eur. J. Phys.* **6** (2008) no. 3, 697–703.
- [10] P. E. T. Jorgensen and R. T. Powers, Positive elements in the algebra of the quantum moment problem, *Probab. Theory Relat. Fields* **99** (1991), no.2, 131–139.
- [11] D. Kang, E. Won, Precise numerical solutions of potential problems using Crank-Nicholson Method, *J. Comput. Phys.* **227** (2008) 2970–2976.
- [12] I. Klep and J. Povh, Semidefinite programming and sums of hermitian squares of noncommutative polynomials, *J. Pure Appl. Algebra* **214** (2010), 740–749.
- [13] J. B. Lasserre, Global optimization with polynomials and the problem of moments, *SIAM J. Optim.* **11** (2000/01), no. 3, 796–817.
- [14] M. Laurent, Sums of squares, moment matrices and optimization over polynomials, *Emerging applications of algebraic geometry*, 157–270, IMA Vol. Math. Appl., 149, Springer, New York, 2009.
- [15] J. Löfberg, Yalmip : A toolbox for modeling and optimization in MATLAB, *Proceedings of the CACSD Conference*, Taipei, Taiwan, 2004. [Online]. Available: <http://control.ee.ethz.ch/~joloef/yalmip.php>
- [16] M. Marletta, A. Zettl, The Friedrichs extension of singular differential operators, *J. Differential Equations* **160** (2000), no. 2, 404–421.

- [17] M. Marshall, *Positive polynomials and sums of squares*, Mathematical Surveys and Monographs, 146. American Mathematical Society, Providence, RI, 2008.
- [18] A. Naftalevich, M. Schreiber, Trigonometric polynomials and sums of squares, Number theory (New York, 1983–84), 225–238, Lecture Notes in Math., 1135, Springer, Berlin, 1985.
- [19] J. Nahas, On the Positivstellensatz in Weyl’s algebra, Proc. Amer. Math. Soc. **138** (2010), 987–995.
- [20] A. Pankov, *Introduction to spectral theory of Schrödinger operators*, <http://www.emis.de/journals/AMEN/posters/pankov.pdf>
- [21] P. A. Parrilo, Semidefinite programming relaxations for semialgebraic problems, Algebraic and geometric methods in discrete optimization. Math. Program. **96** (2003), no. 2, Ser. B, 293–320.
- [22] H. Peyrla, P. A. Parrilo, Computing sum of squares decompositions with rational coefficients, Theor. Comput. Sci. **409** (2008), no. 2, 269–281.
- [23] S. Pironio, M. Navascues, A. Acin, Convergent relaxations of polynomial optimization problems with non-commuting variables, arXiv:0903.4368v1.
- [24] S. Prajna, A. Papachristodoulou, P. Seiler, P. A. Parrilo, SOSTOOLS and its control applications. *Positive polynomials in control*, 273–292, Lecture Notes in Control and Inform. Sci., 312, Springer, Berlin, 2005.
- [25] B. Reznick, Extremal psd forms with few terms, Duke Math. J. **45** (1978) 363–374.
- [26] B. Reznick, Uniform denominators in Hilbert’s Seventeenth Problem, Math. Z. **220** (1995), 75–98.
- [27] W. Rudin, *Functional analysis*, McGraw-Hill Series in Higher Mathematics, McGraw-Hill Book Comp, New York, 1973, xiii+ 397 pp. ISBN 0-07-099558-3
- [28] Y. Savchuk, K. Schmüdgen, On unbounded induced representations of $*$ -algebras, arXiv:0806.2428v1.
- [29] K. Schmüdgen, *Unbounded operator algebras and representation theory*, Operator Theory: Advances and Applications, 37. Birkhuser Verlag, Basel, 1990. 380 pp. ISBN: 3-7643-2321-3
- [30] K. Schmüdgen, A strict Positivstellensatz for the Weyl algebra, Math. Ann. **331** (2005), 779–794.
- [31] K. Schmüdgen, A strict positivstellensatz for enveloping algebras, Math. Z. **254** (2006), no. 3, 641–653.
- [32] K. Schmüdgen, Noncommutative real algebraic geometry-some basic concepts and first ideas, *Emerging applications of algebraic geometry*, 325–350, IMA Vol. Math. Appl., 149, Springer, New York, 2009.
- [33] K. Schmüdgen, Algebras of Fractions and Strict Positivstellensatz for $*$ -Algebras, arXiv:0903.2708v1
- [34] N. Z. Shor, *Nondifferentiable optimization and polynomial problems.*, Nonconvex Optimization and its Applications, 24. Kluwer Academic Publishers, Dordrecht, 1998. xviii+394 pp. ISBN: 0-7923-4997-0
- [35] Jos F. Sturm, Using SeDuMi 1.02, a MATLAB toolbox for optimization over symmetric cones. Interior point methods. Optim. Methods Softw. **11/12** (1999), no. 1-4, 625–653. Available: <http://sedumi.ie.lehigh.edu/>
- [36] R. H. Tütüncü, K. C. Toh, M. J. Todd, Solving semidefinite-quadratic-linear programs using SDPT3. Computational semidefinite and second order cone

programming: the state of the art. Math. Program. **95** (2003), no. 2, Ser. B, 189–217. Available: <http://www.math.nus.edu.sg/~mattohkc/sdpt3.html>

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